

ABSTRACT OF THE DISCLOSURE

A method of finding 3D similarities in protein structures of a first molecule and a second molecule. The method comprises providing preselected information regarding the first molecule and the second molecule. Comparing the first molecule and the second molecule using Longest Continuous Segments (LCS) analysis. Comparing the first molecule and the second molecule using Global Distance Test (GDT) analysis. Comparing the first molecule and the second molecule using Local Global Alignment Scoring function (LGA_S) analysis. Verifying constructed alignment and repeating the steps to find the regions of 3D similarities in protein structures.